

1 2 3 4 5 6 22 23 24 25 26 27

chain bonds :

 $1 - 10 \quad 2 - 13 \quad 3 - 14 \quad 4 - 7 \quad 5 - 12 \quad 6 - 11 \quad 7 - 8 \quad 7 - 9 \quad 8 - 21 \quad 15 - 16 \quad 15 - 18 \quad 16 - 17 \quad 22 - 31 \quad 23 - 34 \quad 24 - 35 \quad 24 - 3$ 25-28 26-33 27-32 28-29 28-30 29-36 36-37 37-38 ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27 exact/norm bonds :

7-8 7-9 28-29 28-30 exact bonds :

 $1 - 10 \quad 2 - 13 \quad 3 - 14 \quad 4 - 7 \quad 5 - 12 \quad 6 - 11 \quad 8 - 21 \quad 15 - 16 \quad 15 - 18 \quad 16 - 17 \quad 22 - 31 \quad 23 - 34 \quad 24 - 35 \quad 25 - 28 \quad 26 - 33 \quad 27 - 28 \quad 28 - 28 \quad 28$ 27-32 29-36 36-37 37-38 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 22-23 22-27 23-24 24-25 25-26 26-27

Match level : 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS

33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS fragments assigned product role: containing 22

fragments assigned reactant/reagent role: containing 1

containing 15